UCRL-JC-120342 Abs & Ext Sum

On the Relationship of Minimal Conditions to Low Density Material Microstructures

Richard M. Christensen

Lawrence Livermore National Laboratory
P. O. Box 808, Livermore, CA 94550 USA

Abstract

A minimal problem is formulated for determining the microstructure of open celled, low density materials. The term microstructure means the manner of connectivity of the sparse population of material members in 3-space. A rigorous solution is found for the minimal problem and it takes the form of diamond cubic symmetry. Thus, the minimal microstructure takes a crystalline form of the diamond cubic type. An approximate approach is followed to determine characteristics of the corresponding amorphous microstructure. The form of the solution in the amorphous case is then used to deduce some characteristics for the associated mechanical properties.

*Work was performed under the auspices of the U.S. DOE for the Lawrence Livermore National Laboratory under contract W-7405-Eng-48.

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Extended Summary

The problem of minimal surfaces is classical. Lord Kelvin (1887) gave a solution for a cellular construct that stood for over 100 years. However, the problem goes back even beyond Kelvin to Plateau and interest in soap films dominated by surface tension. One might expect that such an old problem would be unlikely to yield to new approaches, but such is not the case. Recent results have replaced Kelvin's solution and given valuable new insights, this is the solution of Weaire and Phelan (1994).

The purpose of the present work is to see if the cellular minimal surface problem and solution can be modified and adapted to some contemporary problems of materials science. The specific application is to low density materials, and the objective is the determination of the minimal cellular microstructure for open celled, low density materials. The first step is to briefly outline the classical problem of the minimal surface cellular form, applicable to closed cell materials, thereafter the open cell case will be taken up. Lord Kelvin (1887) gave F = 14 for a truncated octahedron as the proposed minimal area of faces form which then in cellular form results in cubic symmetry. Weaire and Phelan (1994) have recently revealed a completely unexpected and insightful result which has a lower surface content than Kelvin's form, still retaining cubic symmetry. This microstructure is composed of 14 faced cells having 12 pentagons and 2 hexagons combined with cells of regular dodecahedra, the two cell types being in the ratio of 3 to 1 respectively. This is the current status for the closed cell microstructure formulated as a minimal problem.

It is necessary to completely reformulate the minimal problem for application to open celled, low density materials. This problem is derived in a form best described as that of a minimal length problem corresponding to the total length of the material members forming the microstructure, all expressed in suitably

non-dimensionalized form. The end result is a quantified measure, ζ, given in the table below for various cell types.

Minimal Length Problem

Cell Type	Faces, F	$\frac{L}{(VC)^{1/3}}$	η	ζ
Diamond Cubic	4	8.2	1/3	1.66
Simple Cubic	6	12	1/4	1.73
Weaire Phelan Form	13-1/2	16.0	1/3	2.31
Kelvin Form	14	16.0	1/3	2.31
Rhombic Dodecahedron	12	16.5	1/3	2.34

The cells are the standard space filling forms plus the newly described cell of Weaire and Phelan. It is seen that the diamond cubic cell is the minimal value for the cells considered. The diamond cubic cell is in fact the minimal form since it is the only cell type possessing all tetrahedral angles for and with straight edges. In loosely descriptive terms it can be said that the classical minimal surface cell is the "smoothest" form that packs in 3 space, favoring relatively large number of faces, F. In contrast, the minimal length cell is found to be the "least smooth" form that packs in 3 space and thus favors small F, specifically the F = 4 of diamond cubic.

In the present context, amorphous low density materials are taken as materials with microstructures that have a sufficiently high degree of disorder as to not be classifiable into one of the symmetry classes of crystallography, and also to provide isotropy of the mechanical properties. It is found that the amorphous microstructure contains junctions or joints where three material members meet, and junctions were four material members meet, called J_3 and J_4 junctions.

With many of the junctions as J_3's there is a strong disruption of a network of tetrahedral J_4's and the presence of the J_3's effectively destroys the diamond cubic symmetry. It is likely that both of the isotropic properties of the amorphous state become completely controlled by the bending type deformation of the micromembers when under load. This is because of the disruption of the local

tetrahedral symmetry of the diamond cubic form. The shear and volumetric mechanical properties would then be given by

$$\frac{\mu}{E_m} \cong \left(\frac{\rho}{\rho_m}\right)^2$$

$$\frac{k}{E_m} \cong \left(\frac{\rho}{\rho_m}\right)^2$$

where ρ is the low density material density and ρ_m is the composing material density, μ and k are the shear and bulk moduli respectively and E_m is the composing material Young's modulus. Some numerical front factors would also appear.

The dependence upon $(\rho/\rho_m)^2$ rather than the (ρ/ρ_m) dependence of direct resistance of material members results from the expected bending mechanism of the amorphous microstructure. This does not mean that low density material microstructures cannot exist that have a (ρ/ρ_m) dependence, but it does mean that amorphous microstructures formed and dominated by minimal conditions are likely to be bending dominated in their mechanical resistance. This result is in accordance with the observations of Gibson and Ashby (1982) in their pioneering work on low density materials.

References

Gibson, L.J. and Ashby, M.F. (1982), "The Mechanics of Three-Dimensional Cellular Materials," Pro. R. Soc. Lond., 382, 43-59.

Kelvin, Lord (Sir William Thomson) (1887) "On the Division of Space With Minimum Partitional Area," Phil. Mag., 24, 503-514.

Weaire, D. and Phelan, R. (1994), "A Counter-Example to Kelvin's Conjecture on Minimal Surfaces," Phil. Mag. Lett., 69, 107-110.

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